Numerical evaluations of Lindhard's theory of stopping power for a charged particle in a free-electron gas

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Stopping powers derivable from Lindhard's dielectric theory of stopping for a charged particle in a uniform electron gas are calculated as a continuous function of electron density for a wide variety of projectile energies ranging from 10^2 to 10^4 keV/amu. Results are presented for electron densities varying from 10^{22} to 10^{32} electrons/cm^3, a range which includes electron densities generally found for the energy bands of solids and for the atomic levels of atoms.

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INTRODUCTION

Lindhard[1] presented an elegant dielectric formulation of stopping theory for a charged particle penetrating a free-electron gas. His work probably stands as the most complete "first principles" description of energy-loss theory to date.

The original work of Lindhard was later expanded by Lindhard and Winther[2] (L-W) who obtained analytic forms for the stopping power in the limit of high and low projectile velocity relative to the electron gas Fermi velocity. This expansion into analytic expressions was necessary to avoid the significant computational difficulties implicit in the original Lindhard formalism. They also presented results obtained from a direct numerical integration of the Lindhard stopping equation for six different electron densities spanning several decades in value.

In this paper, results of the numerical integration of Lindhard's original stopping equations are presented in detail. Further, polynomial fits of the results are presented so that the Lindhard stopping power can be obtained directly for a given electron charge density. These results are presented as a function of electron density so as to facilitate the calculation of stopping powers with the local density approximation (an approximation in which each volume element of a target is considered to be an electron gas of uniform density; then the total electronic stopping power is obtained by an appropriate averaging over the spatial variation in target electron charge distribution).

LINHARD'S THEORY OF STOPPING POWER

For an ion of charge ze moving with velocity v in a medium of uniform density ρ, the energy loss due to electron excitation can conveniently be written in the form

$$-\frac{dE}{dx}=\frac{4\pi}{m}\left(\frac{ze^2}{v}\right)^2\rho L(\rho,v), \tag{1}$$

where L is called the stopping number and m is the mass of electron. In the dielectric formalism, L is written as

$$L=\frac{i}{\pi\omega_0^2}\int_0^\infty\frac{dk}{k}\int_{-kv}^{kv}\omega\,d\omega\,[\epsilon^{-1}(k,\omega)-1], \tag{2}$$

where ω_0 is the plasma frequency

$$\omega_0^2=\frac{4\pi e^2\rho}{m} \tag{3}$$

and $\epsilon(k,\omega)$ is the wave-number- and frequency-dependent longitudinal dielectric constant.

Lindhard obtained the dielectric constant for a free-electron gas within first-order perturbation theory to be

$$\epsilon(k,\omega)=1+\frac{8\pi me^2}{\hbar^2k^2}\sum_n F(E_n)\left(\frac{1}{k^2+2\mathbf{k}\cdot\mathbf{k}_n-(2m/\hbar^2)(\omega+i\gamma)}+\frac{1}{k^2-2\mathbf{k}\cdot\mathbf{k}_n+(2m/\hbar^2)(\omega+i\gamma)}\right), \tag{4}$$

where E_n and $\mathbf{k}_n$ represent the energy and wave vector for an electron in the nth state and γ is a small positive value. For a free-electron gas at zero temperature,

$$F(E_n)=1 \quad \text{for } E_n<E_F$$

$$=0 \quad \text{for } E_n>E_F \tag{5}$$

and the summation in Eq. (4) can be evaluated to get

$$\epsilon(u,z)=1+(\chi^2/z^2)[f_1(u,z)+if_2(u,z)], \tag{6}$$

where

$$f_1(u,z)=\frac{1}{2}+\frac{1}{8z}[1-(z-u)^2]\left|\ln\frac{z-u+1}{z-u-1}\right|+\frac{1}{8z}[1-(z+u)^2]\left|\ln\frac{z+u+1}{z+u-1}\right|, \tag{7a}$$

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TABLE I. Tabulation of the A_i coefficients in Eq. (16) for $V_{ion} \leq V_F$, where V_F is the Fermi velocity defined by Eq. (9), and for various projectile energies.

Energy (MeV)	$A_0 \times 10^{-1}$	$A_1 \times 10^{0}$	$A_2 \times 10^{0}$	$A_3 \times 10^{0}$	$A_4 \times 10^{0}$
0.1	− 5.229	4.526	− 1.078	9.599	− 3.268
0.2	− 8.132	6.293	− 1.467	13.39	− 4.651
0.3	− 11.96	8.574	− 1.968	18.26	− 6.425
0.4	− 10.36	7.641	− 1.759	16.19	− 5.661
0.5	- 29.12	18.67	− 4.178	39.73	− 14.23
0.6	− 16.1	11.01	− 2.491	23.26	− 8.215
0.7	− 24.54	15.94	− 3.567	33.66	− 11.97
0.8	− 46.47	28.77	− 6.370	60.82	− 21.82
1.0	− 23.79	15.48	− 3.453	32.46	− 11.50
2.0	− 93.14	55.58	− 12.12	115.5	− 41.31
3.0	− 107.1	63.42	− 13.76	130.7	− 46.56
4.0	− 76.02	45.32	− 9.815	92.63	− 32.82
5.0	− 168.1	98.06	− 21.12	200.2	− 71.13
6.0	− 83.91	49.65	− 10.70	100.6	− 35.51
7.0	− 154.7	90.02	− 19.31	182.2	− 64.43
8.0	− 229.9	132.9	− 28.45	268.7	− 9510
10.0	− 144.3	83.73	− 17.89	168.0	− 59.15

and

$$f_2(u,z) \doteq \tfrac{1}{2}\pi u, \quad \text{for } z+u<1$$

$$= (\pi/8z)[1-(z-u)^2] \quad \text{for } |z-u|<1<z+u$$

$$= 0 \quad \text{for } |z-u| \geq 1. \tag{7b}$$

Here the variables k and ω have been replaced by reduced variables

$$z = k/2k_F \quad \text{and} \quad u = \omega/kv_F, \tag{8}$$

where k_F and v_F are defined by

$$E_F = \frac{1}{2}mv_F^2 \equiv \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}(3\pi^2\rho)^{2/3}. \tag{9}$$

In addition, the parameter χ^2 in Eq. (6) is defined by

$$\chi^2 = v_0/\pi v_F, \tag{10}$$

where $v_0 = e^2/\hbar$, the Bohr velocity. When the dielectric constant of Eq. (6) is substituted into Eq. (2), one obtains

$$L = \frac{6}{\pi}\int_0^{v/v_F} u\,du \int_0^{\infty} dz \times \frac{z^3 f_2(u,z)}{[z^2+\chi^2 f_1(u,z)]^2 + [\chi^2 f_2(u,z)]^2}. \tag{11}$$

This expression for L in Eq. (11) is the Lindhard stopping number. For simplicity in integrating the z dependence in Eq. (11), we let $z = u + a$ for a fixed u and factor out $(1/\chi^2)$ to get

$$L = \frac{6}{\pi\chi^2}\int_0^{v/v_F} u\,du \int_u^1 (u+a)^3 F(u,a)\,da, \tag{12}$$

TABLE II. Tabulation of the A_i coefficients in Eq. (16) for $V_{ion} > V_F$, where V_F is the Fermi velocity defined by Eq. (9), and for various projectile energies.

Energy (MeV)	$A_0 \times 10^{-7}$	$A_1 \times 10^{-6}$	$A_2 \times 10^{-5}$	$A_3 \times 10^{-4}$	$A_4 \times 10^{-1}$	$A_5 \times 10^{0}$	$A_6 \times 10^{2}$	$A_7 \times 10^{4}$	$A_8 \times 10^{7}$
0.1	− 244.8	371.9	− 247.0	93.73	− 2221	336.7	− 318.9	172.5	− 407.9
0.2	− 247.3	366.2	− 237.2	87.77	− 2029	299.9	− 277.1	146.2	− 337.3
0.3	− 158.1	232.5	− 149.5	54.91	− 1260	184.8	− 169.4	88.71	− 203.1
0.4	− 90.85	132.9	− 84.96	31.03	− 707.7	103.3	− 94.10	48.97	− 111.4
0.5	− 85.82	125.1	− 79.69	29.00	− 659.1	95.81	− 87.00	45.11	− 102.3
0.6	− 41.18	59.71	− 37.84	13.70	− 309.5	44.74	− 40.38	20.81	− 46.89
0.7	− 52.28	75.71	− 47.93	17.33	− 391.3	56.51	− 50.96	26.25	− 59.09
0.8	− 33.78	48.81	− 30.83	11.12	− 250.3	36.05	− 32.42	16.65	− 37.37
1.0	0.8278	− 1.550	1.209	− 0.5216	13.73	− 2.272	2.316	− 1.333	3.327
2.0	− 0.5526	0.5599	− 0.2033	0.0192	0.7829	− 28.74	4.151	− 0.2934	0.8381
3.0	2.114	− 3.161	2.063	− 0.7676	17.82	− 2.643	2.445	− 1.290	2.973
4.0	0.6460	− 1.025	0.7039	− 0.2740	6.618	− 1.016	0.9700	− 0.5262	1.243
5.0	5.541	− 7.965	5.004	− 1.795	40.21	− 5.758	5.150	− 2.629	5.867
6.0	8.225	− 11.76	7.345	− 2.620	58.35	− 8.310	7.389	− 3.751	8.324
7.0	3.808	− 5.453	3.413	− 1.219	27.20	− 3.880	3.456	− 1.757	3.904
8.0	5.177	− 7.381	4.599	− 1.636	36.34	− 5.160	4.575	− 2.315	5.121
10	6.605	− 9.366	5.804	− 2.053	45.35	− 6.404	5.646	− 2.842	6.250

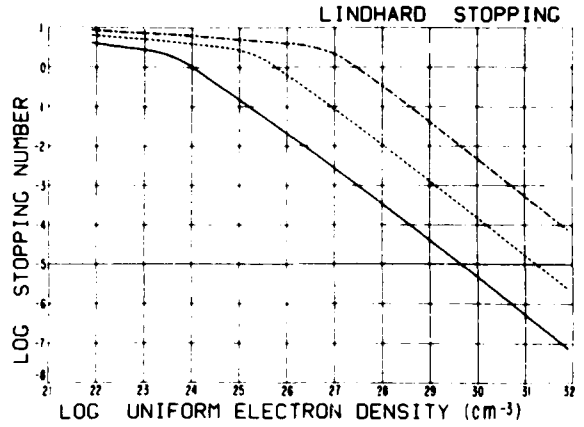

FIG. 1. Plot of variation in stopping number [Eq. (12)] with electron density for select projectile energies. [(—) 100 keV/amu; (- - - -) 1000 keV/amu; (- - - -) 10 000 keV/amu].

where

$$F(u,a) = \frac{\chi^2 f_2(u,a)}{g^2(u,a) + [\chi^2 f_2(u,a)]^2} \tag{13a}$$

and

$$g(u,a) = (u+a)^2 + \chi^2 f_1(u,a). \tag{13b}$$

In Eq. (13a), $f_1(u,a)$ is defined by Eq. (7a) with $z = u + a$ and $f_2(u,a)$ is given by

$$f_2(u,a) = \tfrac{1}{2}\pi u \quad \text{for } 2u + a < 1 \tag{14a}$$

$$= \frac{\pi(1-a^2)}{8(u+a)} \quad \text{for } |a| a < 1 < 2u + a \tag{14b}$$

$$= 0 \quad \text{for } |a| > 1 \tag{14c}$$

The contributions to Eq. (12) arising from regions $2u + a < 1$ and $|a| < 1 < 2u + a$ are straightforward to evaluate. The contribution to Eq. (12) arising from the region $|a| > 1$ is somewhat tricky when $g(u,a) = 0$. In this case,

$$\lim_{f \to 0} F(u,a) = \pi\delta[g(u,a)]$$

$$\equiv \pi\delta[a - a_0(u)] \left|\frac{\partial g}{\partial a}\right|^{-1}_{a_0(u)}, \tag{15}$$

where $a_0(u)$ is the solution to $g(u,a) = 0$ for a fixed u. Thus, when $|a| > 1$, the use of Eq. (15) in Eq. (12) reduces the double integral to a line integral.

We present the result of the numerical integration of Eq. (12) for 100 electron density values in the interval 10^{22}–10^{32} electrons/cm^3 and for projectile energies in the range between 100 and 10^4 keV/amu. The results are presented in a "least-squares" polynomial fit of stopping number with electron density in the form

$$L = \exp\left\{\sum_{i=0}^{n} A_i \left[\ln \rho\left(\frac{\bar{e}}{\text{cm}^3}\right)\right]^i\right\}, \tag{16}$$

where the A_i and n are given in Tables I and II. The polynomial fit is presented in two parts, one for $v_{\text{ion}} < v_F$, and one for $v_{\text{ion}} > v_F$, where v_F is the Fermi velocity defined by Eq. (9). Typically illustrations of the variation in stopping number with electron density and energy can be found in Fig. 1.

SUMMARY

We have presented the results of the numerical integration of Lindhard's stopping number over a wide range of electron densities and projectile energies. The results are given in the form of a polynomial fit of stopping number with electron density. The results of this paper will subsequently be used to apply the Lindhard theory of stopping to "real" solids via the use of the local density approximation.

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